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Multiparameter correlations for describing thermodynamic parameters of solvation: II. Enthalpy of specific interaction

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Abstract

The applicability of the approach based on the linear solvation energy relationship to describing the enthalpies of specific solvent-solute interactions was examined. In associated solvents, this approach reflects the contribution of specific interaction incorrectly. Although the enthalpies of solvation as a whole are described well, this is an "occasional" result and is due to averaging over different compounds and redistribution of contributions from other types of interactions. A modification of this approach was suggested to take into account the effect of reorganization of an associated solvent.

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